C:\Program Files\STNEXP\Queries\10 614362 Elected NK1 Antagonist.str chain nodes : 13 15 16 17 18 19 20 21 22 23 24 25 26 27 28 34 35 36 37 38 39 40

ring nodes: 1 2 3 4 5 6 7 8 9 10 11 12 14 29 30 31 32 33

4-13 8-20 10-21 12-25 13-14 13-15 15-16 15-17 17-18 17-19 19-20 21-22 21-23 21-24 25-26 25-27 25-28 31-34 34-35 34-36 36-37 37-38 38-39 39-40 ring bonds :

g bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 14-29 14-33 29-30 30-31 31-32 32-33

exact/norm bonds: 13-14 14-29 14-33 15-16 15-17 17-18 17-19 29-30 30-31 31-32 31-34 32-33 34-35 34-36 38-39

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 isolated ring systems : containing 1 7 : 14 :

Match level :

chain bonds :

1.htcm 2:Atcm 3:Atcm 4:Atcm 5:Atcm 6:Atcm 7:Atcm 8:Atcm 9:Atcm 10:Atcm 11:Atcm 11:Atcm 12:Atcm 11:CLASS 13:CLASS 19:CLASS 19:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS 23:CLASS 25:CLASS 25:CLAS